App 's

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN 2002:428911 CAPLUS

DN 137:6205

TI Preparation of benzazepinones, isoquinolinones and related compounds as inhibitors of poly(ADP-ribose) polymerase (PARP) for the prevention and/or treatment of tissue damage from cell trauma or cell death due to necrosis or apoptosis.

IN Ferraris, Dana V.; Li, Jia-He; Kalish, Vincent J.; Zhang, Jie

PA Guilford Pharmaceuticals Inc., USA

SO PCT Int. Appl., 152 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

1121.	PATENT NO.				KIND DATE					A	PPLI	CATI	ON N	0.	DATE				
ΡI	WO	2002044183			A	2	20020606			W	20	01-U	S448	 15	20011130				
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			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	NZ,	PH,	PL,	
			PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	
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			CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	
			BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG	
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	US	2003	0228	83	A.	1	20030130			U:	S 20	01-9	9677	6	20011130				
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	US	2001	-310	274P	P		2001	0809											
	WO	2001	-US4	4815	W		2001	1130											
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AB This invention discloses the prepn. of title compds. I and II, their pharmaceutically acceptable salts, and related compds. as inhibitors of poly(ADP-ribose) polymerase (PARP) [wherein: A = N, C, CH2, CH; B = C, N, NH, S, SO, SO2; X = C, CH, N; Y = C, N; Z = C, CH2, N, CO; provided that at least one of X, Y, or Z is N; R1, R2, R3, R5 when present are optionally or independently = H, OH, :O, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, halogen, amine, COR8 (R8 = H, OH, (un)substituted alkyl,

alkenyl, alkynyl, alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl, heteroaryl), OR6, NR6R7 (R6, R7 independently = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl); R1, R2, R3, R5 optionally form ring through a straight or branched C1-4alkyl which may addnl. contain 1-2 double or triple bonds; R4 = 1-3 of H, halo, or alkyl; with proviso that when A, X, or Z = C, then R1, R2, R3 when present may also independently = halogen, CN, O; R9, R10, R11, R12 optionally or independently = H, halogen, amino, OH, halo-amine, O-alkyl, O-aryl, (un) substituted alkyl, alkenyl, alkynyl, alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, COR8; R13 = 1-3 of H, halogen, alkoxy, alkyl]. For example, cyclocondensation of formylindazole III (prepd. from Me indole-4-carboxylate and NaNO2/AcOH), with hydrazine provided claimed benzoazulenone IV as a white solid. Benzoazulenone IV inhibited human recombinant PARP at an IC50 of 0.018 .mu.M. PARP IC50 inhibition studies for an addnl. 156 examples are provided, ranging in values from 0.01 to 20 .mu.M. data are provided for the in vivo treatment of focal cerebral ischemia and gout via PARP inhibition with selected compds. II. The present invention is believed to protect cells, tissue and organs against the ill-effects of reactive free radicals and nitric oxide through inhibition of PARP activity.

IT 433726-67-1P 433726-71-7P 433726-76-2P 433726-79-5P 433726-80-8P 433726-81-9P 433726-86-4P 433727-89-0P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzazepinones, isoquinolinones and related compds. as inhibitors of poly(ADP-ribose) polymerase (PARP)) 433726-67-1 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-methoxy- (9CI) (CA INDEX NAME)

RN

RN 433726-71-7 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 433726-76-2 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 433726-79-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-

2-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 433726-80-8 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 433726-81-9 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-amino- (9CI) (CA INDEX NAME)

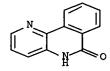
Absolute stereochemistry.

RN 433727-89-0 CAPLUS
CN 2,5-Diazabicyclo[2.2.1]heptane-2-carboxylic acid, 5-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-, 1,1-dimethylethyl ester, (1S,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT **94191-07-8P**, Benzo[c]-1,5-naphthyridin-6(5H)-one

433726-68-2P 433726-69-3P 433726-70-6P 433726-72-8P 433726-73-9P 433726-74-0P 433726-75-1P 433726-77-3P 433726-78-4P 433726-82-0P 433726-83-1P 433726-84-2P 433726-85-3P 433726-87-5P 433726-88-6P 433726-89-7P 433726-90-0P 433727-88-9P 433727-90-3P 433727-91-4P 433727-92-5P 433727-93-6P 433727-94-7P 433727-95-8P 433727-96-9P 433727-97-0P 433727-98-1P 433727-99-2P 433728-00-8P 433728-01-9P 433728-02-0P 433728-03-1P 433728-04-2P 433728-05-3P 433728-06-4P 433728-07-5P 433728-08-6P 433728-09-7P 433728-10-0P 433728-11-1P 433728-12-2P 433728-13-3P 433728-14-4P 433728-15-5P 433728-16-6P 433728-17-7P 433728-18-8P 433728-19-9P 433728-20-2P 433728-21-3P 433728-22-4P 433728-23-5P 433728-24-6P 433728-25-7P 433728-26-8P 433728-27-9P 433728-28-0P 433728-29-1P 433728-31-5P 433728-32-6P 433728-33-7P 433728-34-8P 433728-35-9P 433728-36-0P 433728-37-1P 433728-38-2P 433728-39-3P 433728-40-6P 433728-41-7P 433728-42-8P 433728-43-9P 433728-44-0P 433728-45-1P 433728-46-2P 433728-47-3P 433728-48-4P 433728-50-8P 433728-51-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; prepn. of benzazepinones, isoquinolinones and related compds. as inhibitors of poly(ADP-ribose) polymerase (PARP)) 94191-07-8 CAPLUS Benzo[c]-1,5-naphthyridin-6(5H)-one (9CI) (CA INDEX NAME)



RN

CN

RN 433726-68-2 CAPLUS CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 8-methoxy- (9CI) (CA INDEX NAME)

433726-69-3 CAPLUS RNBenzo[c]-1,5-naphthyridin-6(5H)-one, 2-chloro- (9CI) (CA INDEX NAME)

RN 433726-70-6 CAPLUS

CN Benzo[c]-1,5-naphthyridine-2,6-dione, 1,5-dihydro- (9CI) (CA INDEX NAME)

RN 433726-72-8 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 3-chloro- (9CI) (CA INDEX NAME)

RN 433726-73-9 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 3-amino- (9CI) (CA INDEX NAME)

RN 433726-74-0 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[[2-(4-morpholinyl)ethyl]amino]-(9CI) (CA INDEX NAME)

RN 433726-75-1 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[[3-(diethylamino)propyl]amino]-(9CI) (CA INDEX NAME)

RN 433726-77-3 CAPLUS

CN 2,5-Diazabicyclo[2.2.1]heptane-2-carboxylic acid, 5-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 433726-78-4 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(2,5-diazabicyclo[2.2.1]hept-2-yl)-

(9CI) (CA INDEX NAME)

RN 433726-82-0 CAPLUS

CN Acetamide, 2-chloro-N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-(9CI) (CA INDEX NAME)

RN 433726-83-1 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(4-methyl-4-oxido-1-piperazinyl)-

1-oxide (9CI) (CA INDEX NAME)

RN 433726-84-2 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[4-(1-pyrrolidinyl)-1-

piperidinyl]-

(9CI) (CA INDEX NAME)

RN 433726-85-3 CAPLUS
CN 1-Piperazineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-y1)4-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 433726-89-7 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(4-cyclopentyl-1-piperazinyl)(9CI) (CA INDEX NAME)

RN 433726-90-0 CAPLUS
CN 1-Piperidineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-y1)(9CI) (CA INDEX NAME)

RN 433727-88-9 CAPLUS
CN Benzo[c]-1,5-naphthyridine-2,6-dione, 1,5-dihydro-, monohydrobromide
(9CI)
(CA INDEX NAME)

### HBr

RN 433727-90-3 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(4-methyl-4-oxido-1-piperazinyl)(9CI) (CA INDEX NAME)

RN 433727-91-4 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(4-methyl-1,4-dioxido-1-piperazinyl)- (9CI) (CA INDEX NAME)

RN 433727-92-5 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[4-(cyclopropylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 433727-93-6 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-methyl-2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433727-94-7 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-(cyclopropylmethyl)-2,5diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

RN 433727-95-8 CAPLUS

CN 2,5-Diazabicyclo[2.2.1]heptane-2-acetonitrile, 5-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-, (1S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433727-96-9 CAPLUS

CN 2,5-Diazabicyclo[2.2.1]heptane-2-acetic acid, 5-(5,6-dihydro-6-oxobenzo[c]-

1,5-naphthyridin-2-yl)-, ethyl ester, (1S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433727-97-0 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(2,5-dimethylphenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA)

INDEX

NAME)

Absolute stereochemistry.

RN 433727-98-1 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(4-fluorophenyl)methyl]2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433727-99-2 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(4-methoxyphenyl)methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433728-02-0 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(2-fluorophenyl)methyl]-

2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433728-03-1 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(3-methylphenyl)methyl]-

2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433728-04-2 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(3-chlorophenyl)methyl]-

2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

RN 433728-05-3 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(2-methylphenyl)methyl]2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433728-06-4 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(2-chlorophenyl)methyl]2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

RN 433728-07-5 CAPLUS
CN Benzoic acid, 4-[[(15,4s)-5-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2yl)-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433728-08-6 CAPLUS
CN Benzoic acid, 3-[[(1s,4s)-5-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2yl)-2,5-diazabicyclo[2.2.1]hept-2-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433728-09-7 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(4-methylphenyl)methyl]2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

RN 433728-10-0 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[[4-(phenylmethoxy)phenyl]methyl]-2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433728-11-1 CAPLUS
CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[(1S,4S)-5-[(3-fluorophenyl)methyl]2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 433728-12-2 CAPLUS CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[4-(2-pyridinylmethyl)-1piperazinyl] - (9CI) (CA INDEX NAME)

RN 433728-13-3 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-[4-(3-pyridinylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

RN 433728-14-4 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-2-(dimethylamino)-, hydrochloride (5:6) (9CI) (CA INDEX NAME)

●6/5 HCl

RN 433728-15-5 CAPLUS
CN 1-Piperidineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-y1), monohydrochloride (9CI) (CA INDEX NAME)

RN 433728-16-6 CAPLUS
CN 1-Piperidineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)4-(1-pyrrolidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

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HCl

RN 433728-18-8 CAPLUS
CN 2H-Isoindole-2-acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin2yl)- (9CI) (CA INDEX NAME)

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RN 433728-19-9 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-2-(dipentylamino)- (9CI) (CA INDEX NAME)

RN 433728-20-2 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 433728-21-3 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-2-[(2-phenylethyl)(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 433728-22-4 CAPLUS
CN 1-Piperazineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-y1)4-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)

RN 433728-23-5 CAPLUS
CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)-2-(dipropylamino)- (9CI) (CA INDEX NAME)

RN 433728-24-6 CAPLUS
CN 1-Piperidineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-y1)4-oxo- (9CI) (CA INDEX NAME)

RN 433728-25-7 CAPLUS
CN Acetamide, 2-(dibutylamino)-N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin2-yl)- (9CI) (CA INDEX NAME)

RN 433728-26-8 CAPLUS
CN 4-Morpholineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-2-yl)(9CI) (CA INDEX NAME)

RN 433728-27-9 CAPLUS
CN 1H-Imidazole-1-acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin2yl)- (9CI) (CA INDEX NAME)

RN 433728-28-0 CAPLUS
CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2(dimethylamino)-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 433728-29-1 CAPLUS
CN 1-Piperidineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-y1), hydrochloride (9CI) (CA INDEX NAME)

x HCl

RN 433728-31-5 CAPLUS

CN 1-Piperidineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-

y1)4-(1-pyrrolidiny1)-, dimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 433728-30-4 CMF C23 H27 N5 O2

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 433728-32-6 CAPLUS

CN 1-Piperazineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-

4-(1-methylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 433728-33-7 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[2-(1-pyrrolidinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 433728-34-8 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[3-(1-methyl-2-pyrrolidinyl)propyl]amino]- (9CI) (CA INDEX NAME)

RN 433728-35-9 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[2-(2-pyridinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 433728-36-0 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[2-(3-pyridinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 433728-37-1 CAPLUS

CN 1-Piperazineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-

4-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 433728-38-2 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[2-(4-morpholinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 433728-39-3 CAPLUS

CN Acetamide, 2-[[2-(diethylamino)ethyl]amino]-N-(5,6-dihydro-6-oxobenzo[c]-

1,5-naphthyridin-3-yl)- (9CI) (CA INDEX NAME)

RN 433728-40-6 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[2-(dimethylamino)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 433728-41-7 CAPLUS

CN Acetamide, 2-[[3-(diethylamino)propyl]amino]-N-(5,6-dihydro-6-oxobenzo[c]-

1,5-naphthyridin-3-yl)- (9CI) (CA INDEX NAME)

RN 433728-42-8 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[3-(dimethylamino)propyl]methylamino]- (9CI) (CA INDEX NAME)

RN 433728-43-9 CAPLUS

CN 1H-1,4-Diazepine-1-acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)hexahydro-(9CI) (CA INDEX NAME)

RN 433728-44-0 CAPLUS

CN 1-Piperazineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-4-methyl- (9CI) (CA INDEX NAME)

RN 433728-45-1 CAPLUS

CN 1-Piperazineacetamide, 4-(1,3-benzodioxol-5-ylmethyl)-N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)- (9CI) (CA INDEX NAME)

RN 433728-46-2 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[2-(2-oxo-1-pyrrolidinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 433728-47-3 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-[[2-(1-piperidinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RN 433728-48-4 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 2-(4-methyl-1-piperazinyl)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 433726-76-2 CMF C17 H18 N4 O

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 433728-50-8 CAPLUS

CN Acetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-2-(dimethylamino)- (9CI) (CA INDEX NAME)

RN 433728-51-9 CAPLUS

CN 1-Piperidineacetamide, N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-(9CI) (CA INDEX NAME)

IT 433728-81-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)

(prepn. of benzazepinones, isoquinolinones and related compds. as inhibitors of poly(ADP-ribose) polymerase (PARP))

RN 433728-81-5 CAPLUS

CN Acetamide, 2-chloro-N-(5,6-dihydro-6-oxobenzo[c]-1,5-naphthyridin-3-yl)-(9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN 2001:162346 CAPLUS

DN 134:359384

TI Photoreaction of 2-Halo-N-pyridinylbenzamide: Intramolecular Cyclization Mechanism of Phenyl Radical Assisted with n-Complexation of Chlorine Radical

AU Park, Yong-Tae; Jung, Chang-Hee; Kim, Moon-Sub; Kim, Kwang-Wook; Song, Nam Woong; Kim, Dongho

CS Department of Chemistry, Kyungpook National University, Taegu, 702-701, S. Korea

SO Journal of Organic Chemistry (2001), 66(7), 2197-2206 CODEN: JOCEAH; ISSN: 0022-3263

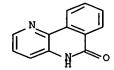
PB American Chemical Society

DT Journal

LA English

GI

The photochem. of 2-halo-N-pyridinylbenzamide I (R = H, Cl, Br; R1 = H, Me; R2 = 4-N-(4-pyridynyl), 3-N-(3-pyridynyl), 2-N-(2-pyridynyl)) and chlorobenzanilide I (R = Cl, R1 = H, R2 = CH) was studied in aq. acetonitrile. The photoreaction of 2-chloro-N-pyridinylbenzamides produced photocyclized products, benzo[c]naphthyridinones in high yield, whereas the bromo analogs produced extensively photoreduced products, pyridinylbenzamides with minor photocyclized product. Since the photocyclization reaction of 2-chloro-N-pyridinylbenzamide was retarded by the presence of oxygen and sensitized by the presence of a triplet sensitizer, acetone or acetophenone, a triplet state of the chloro analog was involved in the reaction. Since several radical intermediates, particularly n-complexes of chlorine radical, were identified in the laser flash photolysis of 2-chloro-N-pyridinylbenzamide, an intramol. cyclization mechanism of Ph radical assisted with n-complexation of chlorine radical for the cyclization reaction was proposed: the triplet state (78 kcal/mol) of the chloro analog, which was populated by the excitation underwent a homolytic cleavage of the C-Cl bond to give Ph and chlorine radicals; while chlorine radical holded the neighbor pyridinyl ring with its n-complexation, the intramol. arylation of the Ph radical with the pyridinyl ring proceeded to produce a conjugated 2,3-dihydropyridinyl radical and then the conjugated radical aromatized to afford a cyclized product, benzo[c]naphthyridinone by ejecting a hydrogen. The photoredn. product can be formed by hydrogen atom abstraction of the Ph .sigma. radical from the environment.



RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN 2000:879316 CAPLUS

DN 134:193358

TI Alkylbenzonaphthyridinones and benzonaphthyridinium quaternary salts

AU Dondela, B.; Sliwa, W.

CS Institute of Chemistry, Pedagogical University, Czestochowa, 42-201,

Pol.

SO Chemistry of Heterocyclic Compounds (New York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2001), Volume Date 2000, 36(7), 830-

836

CODEN: CHCCAL; ISSN: 0009-3122

PB Consultants Bureau

DT Journal

LA English

AB Methyl- and ethylbenzonaphthyridinones, along with ethylbenzonaphthyridinium iodides, 2,5-dimethyl-1,5-benzo[c]naphthyridinium iodide, and isomeric N-(3-bromopropyl)benzonaphthyridinium bromides were synthesized and their structures were confirmed by 1H NMR. Two of the obtained compds. exhibited antibacterial activity.

IT 327096-09-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and antibacterial activity)

RN 327096-09-3 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 5-methyl- (9CI) (CA INDEX NAME)

IT 327096-11-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of benzonaphthyridinones and benzonaphthyridinium salts)

RN 327096-11-7 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one, 5-ethyl- (9CI) (CA INDEX NAME)

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN 1985:45857 CAPLUS

DN 102:45857

TI Palladium-catalyzed cyclization of 2-substituted halogenoarenes by dehydrohalogenation

AU Ames, D. E.; Opalko, A.

CS Chem. Dep., Chelsea Coll., London, SW3 6LX, UK

SO Tetrahedron (1984), 40(10), 1919-25 CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA English

OS CASREACT 102:45857

GI

AB Cyclodehydrohalogenation mediated by Pd catalysts and solvents with different bases (the most satisfactory system being Pd(OAc)2 in AcNMe2 with Na2CO3 as base) has been examd. as a route to some heterocyclic systems. Whereas dehydrogenative cyclization processes require stoichiometric amts. of Pd(II) reagent, the present procedure involves only catalytic amts. (0.1M proportion, or less), of Pd compd. The prepn.

of dibenzofuran, carbazole, fluorenone, phenanthridone, 6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide (I), 6H-dibenzo[b,d]pyran and benzofuran[2,3-b]pyridine derivs. is described. The cyclization of 3-benzamido-2-chloropyridine (II) to 6-hydroxybenzo[c][1,5]naphthyridine (III) illustrates the regiospecificity of the process.

IT 94191-07-8P

RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, by palladium-catalyzed cyclization of benzamidochloropyridine)

RN 94191-07-8 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN 1976:180196 CAPLUS

DN 84:180196

TI 4-Substituted amino-2,6-dioxo-pyrido[3,2-c]isoquinoline derivatives

IN Kobayashi, Goro

PA Kohjin Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

21411 0112 #													
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE								
PI	JP 51011797	A2	19760130	JP 1974-81726	19740718								
	JP 57040832	B4	19820830										
PRAI	JP 1974-81726		19740718										
GI													

AB The pyridoisoquinoline was prepd. by reaction of the methylthio deriv. II with H2NCH2CH(OEt)2. I had sedative and anticonvulsant activities (no data). Thus, fusion of 2 mmoles II with 5 mmoles H2NCH2CH(OEt)2 at 150.degree. for 1 hr gave 85% I.

II

IT 54706-14-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

- RN 54706-14-8 CAPLUS
- CN Benzo[c]-1,5-naphthyridine-3-carbonitrile, 4-[(2,2-diethoxyethyl)amino]-1,2,5,6-tetrahydro-2,6-dioxo-(9CI) (CA INDEX NAME)

# IT 54706-44-4

RL: RCT (Reactant); RACT (Reactant or reagent)

- RN 54706-44-4 CAPLUS
- CN Benzo[c]-1,5-naphthyridine-3-carbonitrile, 1,2,5,6-tetrahydro-4-(methylthio)-2,6-dioxo-(9CI) (CA INDEX NAME)

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L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS
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AN 1975:72760 CAPLUS

DN 82:72760

TI Heterocyclic ketenethioacetal derivatives. IV. Reactions of 1,2,3,4-tetrahydro-1,3-dioxoisoquinoline and 1,2,3,4-tetrahydro-1,4-dioxoisoquinoline with ketenethioacetals and reaction of these products

AU Ueno, Seiichi; Tominaqa, Yoshinori; Matsuda, Yoshiro; Kobayashi, Goro

CS Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan

SO Chemical & Pharmaceutical Bulletin (1974), 22(11), 2624-34 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB Reaction of 1,3-dioxo- or 1,4-dioxo-1,2,3,4-tetrahydroisoquinolines with ketene thioacetals, e.g., (MeS)2C:C(CN)CO2Me, gave the corresponding substitution products, e.g., I, in good yields. The application of these

reactions afforded pyrano[2,3-c]isoquinoline and pyrrolo[1,2-b]isoquinoline, III (Z = O), derivs. The reaction of I and related compds. with amines afforded recyclized products, 2-benzopyrano[3,4-

b]pyridine derivs., e.g. II. The reaction of III (Z = O) with amines gave

amino derivs., e.g., III (Z = NNH2). The reaction of IV with aminoacetal

afforded an aminoacetal deriv. which was treated with HCl to give a cyclized product V. The cyclization of derivs. of III (Z=0) with Et orthoformate or HCO2H gave pyrimidine derivs.

IT 54706-14-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(prepn. and cyclization of)

RN 54706-14-8 CAPLUS

CN Benzo[c]-1,5-naphthyridine-3-carbonitrile, 4-[(2,2-diethoxyethyl)amino]-1,2,5,6-tetrahydro-2,6-dioxo-(9CI) (CA INDEX NAME)

#### IT 54706-44-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(prepn. and reaction with sulfuric acid)

RN 54706-44-4 CAPLUS

CN Benzo[c]-1,5-naphthyridine-3-carbonitrile, 1,2,5,6-tetrahydro-4-(methylthio)-2,6-dioxo-(9CI) (CA INDEX NAME)

IT 54706-45-5P

RN 54706-45-5 CAPLUS

CN Benzo[c]-1,5-naphthyridine-3-carboxamide, 1,2,5,6-tetrahydro-4-(methylthio)-2,6-dioxo-(9CI) (CA INDEX NAME)

## Reference(s):

 Dondela, B.; Sliwa, W., Chem. Heterocycl. Compd. (Engl. Transl.), CODEN: CHCCAL, 36(7), <2000>, 830 - 836, Khim. Geterotsikl. Soedin., CODEN: KGSSAQ(7), <2000>, 944 - 950; BABS-6266153

L7 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

#### Reference(s):

 Dondela, B.; Sliwa, W., Chem. Heterocycl. Compd. (Engl. Transl.), CODEN: CHCCAL, 36(7), <2000>, 830 - 836, Khim. Geterotsikl. Soedin., CODEN: KGSSAQ(7), <2000>, 944 - 950; BABS-6266153

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L10 ANSWER 1 OF 2 MARPAT COPYRIGHT 2003 ACS
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AN 128:180325 MARPAT

TI Preparation of dibenzofuranoxobutyrates and analogs as matrix metalloproteinase inhibitors

IN Sliskovic, Drago Robert; Picard, Joseph Armand

PA Warner-Lambert Company, USA; Sliskovic, Drago Robert; Picard, Joseph Armand

SO PCT Int. Appl., 64 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

GΙ

		PENT			KIND DATE						APPLICATION NO. DATE								
ΡI	WO	9806711			A1 19980219					WO 1997-US12389 19970716									
		W: AL, AU,			BA,	BB,	BG,	BR,	CA,	CN,	CZ,	EE,	GE,	GH,	HU,	IL,	IS,	JP,	
			KR,	LC,	LK,	LR,	LT,	LV,	MG,	MK,	MN,	MX,	NO,	NZ,	PL,	RO,	SG,	SI,	
			SK,	SL,	TR,	TT,	UA,	US,	UZ,	VN,	YU,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	
			RU,	ТJ,	TM														
		RW:	GH,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	
			GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	
			GN,	ML,	MR,	ΝE,	SN,	TD,	TG										
	AU	9737293			Al 19980306					AU 1997-37293 19970716									
	EP	9235	923569			1	19990623			EP 1997-934175					19970716				
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			IE,	SI,	LT,	LV,	FI												
	JP	2000	5166	07	T.	2 :	2000	1212		J	P 19	98-5	0971	2	19970716				
	ZΑ	9707	328		Α		1998	0219		ZA 1997-7328					19970814				
	US	6020	366		A 20000201				U:	S 19	98-1	7183	3	19981027					
PRAI	US	1996	-240	25P	19960816														
	WO 1997-US12389				19	9707	16												

$$R1$$
  $W1$   $Z1$   $R$   $R2$ 

AB Title compds. [I; R = CR6R7CH2CH(NR4R5)COR3; R1, R2 = H, halo, alkyl, alkoxy, etc.; R3 = OH, alkoxy, aryloxy, NHOH, etc.; R4, R5 = H, alkyl, aryl, acyl, etc.; R6 = H and R7 = OH or SH; R6R7 = O, S, NOH, NNH2, etc.;

Y = O, SOO-2, NR1, CH2, (NH)CO, etc.; W,W1,Z,Z1 = CR1 or N] were prepd. Thus, dibenzofuran was acylated by N-trifluoroacetyl-L-aspartic acid anhydride to give (S)-R8COCH2CH(NHCOCF3)CO2H (R8 = 2-dibenzofuranyl). Data for biol. activity of I were given.

MSTR 1A

$$G9 = 8$$

$$G14 = 72-6 73-10$$

$$G15 = 88 / N$$

DER: and pharmaceutically acceptable salts and solvates

MPL: claim 1

STE: and isomers and stereoisomers

# MSTR 1B

$$G9 = 5$$

$$G14 = 72-6 73-10$$

$$G15 = 88 / N$$

88----G3

DER: and pharmaceutically acceptable salts and solvates

MPL: claim 1

STE: and isomers and stereoisomers

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L10 ANSWER 2 OF 2 MARPAT COPYRIGHT 2003 ACS
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AN 120:107044 MARPAT

TI Polycyclic heterocyclic agrochemical fungicides

IN Daub, John Powell; Finkelstein, Bruce Lawrence; Kleier, Daniel Anthony

PA du Pont de Nemours, E. I., and Co., USA

SO PCT Int. Appl., 138 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.				KIND DATE				APPLICATION NO. DATE									
PI	WO	9314080			A1		19930722			WO 1992-US11329 19921230								
		W: AU, BB,		BG,	BR,	CA,	CS,	FI,	HU,	JP,	KP,	KR,	LK,	MG,	MN,	MW,	NO,	
		NZ, PL,		RO,	RU,	SD,	UA,	US										
		RW:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,
			BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML,	MR,	SN,	TD,	TG			
	AU	9334270			A1 19930803				AU 1993-34270 1992123							1230		
	ΕP	623125			A1 19941109				EP 1993-902842						19921230			
		R: DE, DK,			FR, GB													
	CN	1074443			A 19930721			CN 1993-100432						19930115				
PRAI	US	1992-821724			19920115													
	WO	1992-US11329			19	9212	30											

GΙ

AB The title fungicidal compds. I [A = direct bond, (un) substituted bridging group; Q = fused (un) substituted benzene, (un) substituted naphthalene, (un) substituted thiophene, (un) substituted furan, (un) substituted pyrrole, (un) substituted pyridine, (un) substituted pyrimidine ring; Rl-R4 = H, halogen, CN, HO, C1-6 alkyl, C1-4 haloalkyl, C1-4 alkylthio, C1-4 alkylsulfinyl, etc.; X = N, CR4; Y, Z = N, CR5; R5 = H, halogen, C1-2 alkyl, C1-2 alkoxy; the total no. of heteroatoms in ring A are .ltoreq.2] and their agriculturally suitable salts or metal complexes are prepd., and I-contg. formulations presented. Thus, pyrimidine II was prepd. (m.p. 166-166.5.degree.) and demonstrated antifungal activity against a variety of phytopathogenic fungi.

### MSTR 1C

G10 = 41

$$G12 = 70-7 71-2$$

DER: or agriculturally suitable salts or metal complexes

MPL: claim 1

NTE: substitution is restricted

STE: including all geometric and stereoisomers

=> d l1; d his; log y L1 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation.

(FILE 'HOME' ENTERED AT 11:56:51 ON 24 APR 2003)

FILE 'REGISTRY' ENTERED AT 11:57:01 ON 24 APR 2003

L1 STRUCTURE UPLOADED

L2 7 S L1

L3 94 S L1 FUL

FILE 'CAPLUS' ENTERED AT 11:57:28 ON 24 APR 2003

L4 6 S L3

FILE 'BEILSTEIN' ENTERED AT 11:58:01 ON 24 APR 2003

L5 0 S L1

L6 6 S L1 FUL

L7 2 S L6 NOT L3

FILE 'MARPAT' ENTERED AT 11:58:53 ON 24 APR 2003

L8 0 S L1

L9 3 S L1 FUL

L10 2 S L9 NOT L4

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 113.01 366.27

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

ENTRY SESSION

CA SUBSCRIBER PRICE -1.24 -5.15

STN INTERNATIONAL LOGOFF AT 11:59:32 ON 24 APR 2003

L4ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS

AN1985:45857 CAPLUS

DN 102:45857

Palladium-catalyzed cyclization of 2-substituted halogenoarenes by TI dehydrohalogenation

AU Ames, D. E.; Opalko, A.

Chem. Dep., Chelsea Coll., London, SW3 6LX, UK CS

Tetrahedron (1984), 40(10), 1919-25 SO

CODEN: TETRAB; ISSN: 0040-4020

DTJournal

LA English

os CASREACT 102:45857

GI

Cyclodehydrohalogenation mediated by Pd catalysts and solvents with AB different bases (the most satisfactory system being Pd(OAc)2 in AcNMe2 with Na2CO3 as base) has been examd. as a route to some heterocyclic systems. Whereas dehydrogenative cyclization processes require stoichiometric amts. of Pd(II) reagent, the present procedure involves only catalytic amts. (0.1M proportion, or less), of Pd compd. prepn. of dibenzofuran, carbazole, fluorenone, phenanthridone, 6H-dibenzo[c,e][1,2]thiazine 5,5-dioxide (I), 6H-dibenzo[b,d]pyran and benzofuran[2,3-b]pyridine derivs. is described. The cyclization of 3-benzamido-2-chloropyridine (II) to 6-hydroxybenzo[c][1,5]naphthyridine (III) illustrates the regiospecificity of the process.

IT 94191-07-8P

> RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, by palladium-catalyzed cyclization of benzamidochloropyridine)

RN 94191-07-8 CAPLUS

CN Benzo[c]-1,5-naphthyridin-6(5H)-one (9CI) (CA INDEX NAME)

100